

Universal bosonic tetramers of dimer-atom-atom structure

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Unstable four-boson states having an approximate dimer-atom-atom structure are studied using momentum-space integral equations for the four-particle transition operators. For a given Efimov trimer the universal properties of the lowest associated tetramer are determined. The impact of this tetramer on the atom-trimer and dimer-dimer collisions is analyzed. The reliability of the three-body dimer-atom-atom model is studied.

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I. INTRODUCTION

It took more than 30 years till Efimov's prediction for the existence of weakly bound three-particle states with asymptotic discrete scaling symmetry [1] was confirmed in the cold-atom physics experiments [2]. This discovery raised the interest in few-body systems with resonant short-range interactions, both experimentally and theoretically. After the three-body system where semi-analytical results have been obtained as summarized in Ref. [3], the next step in the complexity to explore the Efimov physics is the system of four identical bosons where several numerical studies [4–10] are already available. Although there is no four-boson Efimov effect [11, 12], the properties of the four-boson system are strongly affected by the three-boson Efimov effect. The observables of the four-boson collisions show the same discrete scaling symmetry and are related to the respective trimer binding energies in a universal way provided the size of the involved few-body bound states greatly exceeds the interaction range [6, 9]. Furthermore, below each Efimov trimer in a certain regime there are two tetramers [5, 6]. The tetramers associated with the excited trimers are unstable bound states (UBS) [10, 13, 14] and lead to resonant effects in the four-boson reactions. First numerical calculations of the four-boson recombination [6] and dimer-dimer collisions [15] in the adiabatic hyperspherical representation were followed by the work of Refs. [9, 16, 17] employing the integral equations for the transition operators that were solved in the momentum-space framework. In the latter case the universal limits for the scattering observables and tetramer properties such as widths and intersections with thresholds were obtained with considerably higher accuracy; furthermore, remarkable resonant effects were predicted in the atom-trimer collisions as well [14]. The theoretical results [6, 15–17] are roughly consistent with the existing data from the dimer-dimer and four-atom recombination experiments [18–21] performed in a regime that is not strictly universal.

In the present work we will study a different type of bosonic tetramers, namely, the ones of the approximate dimer-atom-atom structure. Their existence was predicted in Refs. [3, 15] as a consequence of the three-body

Efimov effect in the three-body system made off a dimer and two atoms. This is illustrated in Fig. 1 where we schematically show the four-boson energy (E) spectrum as function of $1/a$ with a being the two-boson scattering length. We consider the regime around the special value $a = a_n^d$ that corresponds to the n th Efimov trimer being at the atom-dimer threshold, i.e., $b_d = b_n$ where b_d (b_n) is the dimer (n th trimer) binding energy relative to the free particle threshold. If the trimer is a true bound state with zero width, i.e., if deeper dimers are absent (which is not the case in typical experiments [18–21]), the atom-dimer scattering length A_d is infinite at $a = a_n^d$. Sufficiently close to $E = -b_n$ and $a = a_n^d$ where A_d greatly exceeds the dimer size being of the order of a , one may expect to mimic some properties of the few-boson systems using a model that considers the dimer as a pointlike particle. Then in the effective three-body system consisting of a dimer and two atoms there are two atom-dimer pairs with infinite two-body scattering length A_d . In such a three-body model of the four-boson system the three-body Efimov effect occurs, however, with a very large discrete scaling factor $e^{\pi/s_0} \approx 2.016 \times 10^5$ [3]. The resulting Efimov states accumulate at $E = -b_d$. Their dimer-atom-atom structure is only an approximation but no attempt has been made so far to describe them rigorously as four-boson states. This will be done in the present work using exact four-particle equations. We label the tetramers of this type by two integers (n, m) where n refers to the associated Efimov trimer and $m = 0, 1, 2, \dots$ distinguishes between different states existing around $a = a_n^d$ with fixed n . The (n, m) th tetramer intersects the n th atom-trimer threshold at $a = a_{n,m}^t$ and the dimer-atom-atom threshold at $a = a_{n,m}^d$. The calculation of these tetramers is technically very difficult task owing their weak binding and very large e^{π/s_0} ; our results will be limited to $m = 0$ states. Furthermore, all these tetramers lie above the dimer-dimer threshold and above all lower atom-trimer thresholds n' with $n' < n$. Therefore the considered tetramers are UBS with finite width. We will extract their properties using rigorous four-particle scattering calculations. Performing in addition the three-body calculations we will establish the limitations of the dimer-atom-atom model.

In Sec. II we shortly recall the technical framework. In Sec. III we present results for tetramer properties and

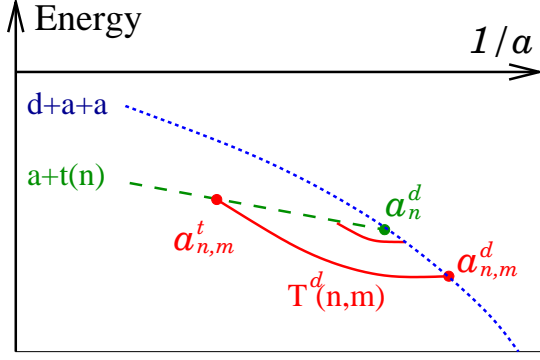


FIG. 1. (Color online) Schematic representation of the four-boson energy spectrum in the vicinity of the dimer-atom-atom (dotted line) and the n th atom-trimer (dashed line) threshold intersection at $a = a_n^d$. The tetramers (solid lines) accumulate at $a = a_n^d$ and $E = -b_d$ but for simplicity only two states ($m = 0, 1$) are displayed; only qualitative relations are preserved. The (n, m) th tetramer intersects the dimer-atom-atom and the n th atom-trimer thresholds at $a = a_{n,m}^d$ and $a = a_{n,m}^t$, respectively.

their effect on the atom-trimer and dimer-dimer scattering observables. We summarize in Sec. IV.

II. FOUR-BOSON SCATTERING EQUATIONS

To describe the collisions in the four-boson system we use exact Alt, Grassberger and Sandhas (AGS) equations [22] for the transition operators $\mathcal{U}_{\beta\alpha}$ in the symmetrized form

$$\mathcal{U}_{11} = P_{34}(G_0 t G_0)^{-1} + P_{34}U_1 G_0 t G_0 \mathcal{U}_{11} + U_2 G_0 t G_0 \mathcal{U}_{21}, \quad (1a)$$

$$\mathcal{U}_{21} = (1 + P_{34})(G_0 t G_0)^{-1} + (1 + P_{34})U_1 G_0 t G_0 \mathcal{U}_{11}, \quad (1b)$$

$$\mathcal{U}_{12} = (G_0 t G_0)^{-1} + P_{34}U_1 G_0 t G_0 \mathcal{U}_{12} + U_2 G_0 t G_0 \mathcal{U}_{22}, \quad (1c)$$

$$\mathcal{U}_{22} = (1 + P_{34})U_1 G_0 t G_0 \mathcal{U}_{12}. \quad (1d)$$

Here G_0 is the free resolvent, P_{34} is the permutation operator of particles 3 and 4, $t = v + v G_0 t$ is the two-particle transition matrix derived from the potential v , and U_α are the symmetrized AGS operators [23] for $3+1$ ($\alpha = 1$) and $2+2$ ($\alpha = 2$) subsystems. We solve the AGS equations (1) in the momentum-space framework using the partial-wave decomposition. In the present study only the states with zero total angular momentum and positive parity (0^+) corresponding to the quantum numbers of the tetramers need to be considered; among them the states with the nonconserved angular momentum of the three-boson subsystem $J \leq 3$ have to be included for the convergence. The atom-atom interaction v is taken over from Ref. [9]; it is given by a separable S -wave potential with one- or two-term gaussian form factors. Further technical details can be found in Refs. [17, 23, 24].

The scattering amplitudes for all elastic and inelastic two-cluster reactions are obtained as the on-shell matrix elements of the AGS transition operators [23]; the amplitudes for breakup and recombination [17] are given by the integrals involving $\mathcal{U}_{\beta\alpha}$.

The unstable tetramers manifest themselves as poles of the operators $\mathcal{U}_{\beta\alpha}$ in the complex energy plane at $-B_{n,m}^d - i\Gamma_{n,m}^d/2$ with $-B_{n,m}^d$ being the energy of the (n, m) th tetramer relative to the four-boson breakup threshold and $\Gamma_{n,m}^d$ being its width. The UBS pole in the complex energy plane is located in one of the unphysical sheets that is adjacent to the physical sheet [13] and affects the physical observables leading to resonant effects in the four-boson scattering. Thus, the properties of the unstable tetramers can be extracted from the behavior of $\mathcal{U}_{\beta\alpha}$ as described in Ref. [14].

In the three-body dimer-atom-atom (3BDAA) model the corresponding reactions are described by solving the AGS three-body scattering equations [25]. These calculations need two pair potentials. The atom-atom potential $v_{aa} = v$ is the same as in full four-boson calculations. The atom-dimer potential v_{ad} is taken in the momentum-space representation as $\langle \mathbf{k}' | v_{ad} | \mathbf{k} \rangle = \exp(-k'^2/\Lambda_d^2) \lambda_d \exp(-k^2/\Lambda_d^2)$. Its strength λ_d and momentum cutoff (inverse range) parameter Λ_d for each a are adjusted to reproduce A_d , $(b_n - b_d)$ and atom-dimer effective range predicted by the original three-boson calculations using v_{aa} . As a consequence, v_{ad} yields an accurate description of the low-energy atom-dimer scattering. We note that the range of v_{ad} with $1/\Lambda_d \approx a$ greatly exceeds the range of v_{aa} that is much smaller than a .

III. RESULTS

Unless stated otherwise, our results refer to rigorous four-boson calculations. We present them as dimensionless ratios that are independent of the short-range interaction details in the universal limit. For this one needs to consider reactions involving highly excited Efimov trimers where the finite-range effects become negligible. As shown in previous calculations [7, 9, 14, 16, 17], $n \geq 3$ is sufficient for high accuracy (note that our nomenclature starts with $n = 0$ for the ground state). This is fully consistent with our present results. For example, for the $(n, 0)$ th tetramer intersection with the corresponding atom-trimer threshold we obtain $a_{3,0}^t/a_3^d \approx 1.609$ and $a_{4,0}^t/a_4^d \approx 1.608$ using one-term form factor in the potential v and $a_{3,0}^t/a_3^d \approx 1.607$ and $a_{4,0}^t/a_4^d \approx 1.608$ using two-term form factor, respectively. Thus, we conclude that for large n the universal ratio is

$$a_{n,0}^t/a_n^d = 1.608(1), \quad (2)$$

corresponding to $A_d/a_{n,0}^t = 5.491(3)$. The calculation of the tetramer intersection with the dimer-atom-atom threshold, $a_{n,0}^d$, turns out to be numerically more complicated and less accurate due to its proximity to a_n^d . We

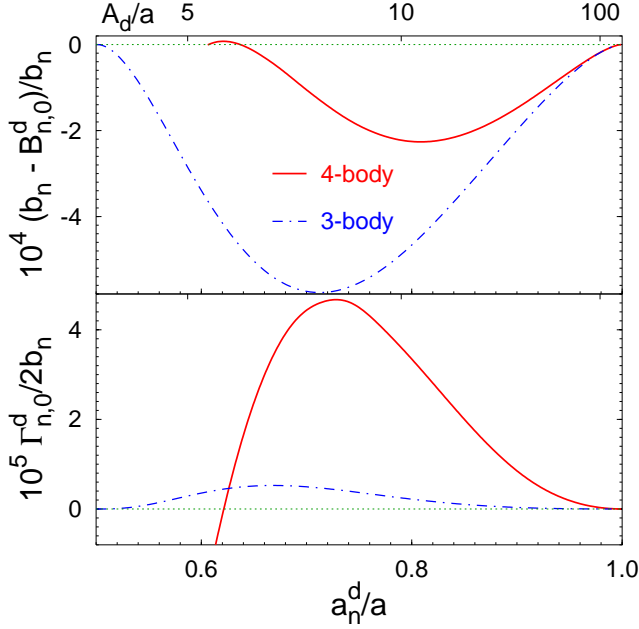


FIG. 2. (Color online) Position of the $(n,0)$ th tetramer relative to the n th atom-trimer threshold (top) and its width (bottom) as functions of the two-boson scattering length a and the atom-dimer scattering length A_d . The results of the full four-body (solid curves) and the 3BDAA (dashed-dotted curves) models are compared. The thin dotted line represents the zero value.

have found that $a_{n,0}^d/a_n^d > 0.9999$. The higher tetramers ($n, m \geq 1$) may exist only at extremely large atom-dimer scattering length A_d , i.e., extremely close to $a = a_n^d$, and cannot be resolved in our four-boson calculations. Thus, with increasing m the ratios $a_{n,m \geq 1}^t/a_n^d$ ($a_{n,m}^d/a_n^d$) very rapidly approach 1 from above (below). For example, our estimations using the 3BDAA model are

$$1 - a_{n,0}^d/a_n^d = 1.2(1) \times 10^{-6}, \quad (3)$$

corresponding to $A_d/a_{n,0}^d = -1.8(1) \times 10^6$, and

$$a_{n,1}^t/a_n^d - 1 = 1.3(1) \times 10^{-6}, \quad (4)$$

corresponding to $A_d/a_{n,1}^t = 1.7(1) \times 10^6$ and $(b_n - b_d)/b_d = 2.6(2) \times 10^{-13}$.

The universal values (2) and (3) indicate that the $(n,0)$ th tetramer as UBS exists at $0.6219 < a_n^d/a < 1.0000012$. We show in Fig. 2 the a -evolution of the $(n,0)$ th tetramer properties, i.e., its relative distance to the n th atom-trimer threshold $(b_n - B_{n,0}^d)/b_n$ and its width $\Gamma_{n,0}^d/2b_n$ as dimensionless universal quantities. We include also the predictions of the 3BDAA model and demonstrate that it is reliable only for the tetramer position at $a_n^d/a > 0.96$ where $|A_d|/a > 50$. Although the 3BDAA model describes well the n th trimer binding and the low-energy atom-dimer scattering, it does not support lower atom-trimer channels and it is obviously not appropriate in the dimer-dimer channel since the 3BDAA

model treats the two dimers asymmetrically. However, these channels are decisive for the tetramer width since in their absence $\Gamma_{n,0}^d$ vanishes. Thus, the failure of the 3BDAA model for $\Gamma_{n,0}^d$ is not surprising. Furthermore, the pointlike dimer approximation may only be reasonable when its size, being of order of a , becomes negligible as compared to $|A_d|$ (that determines also the size of the shallowest trimer if $A_d > 0$), i.e., for $|A_d| \gg a$. Under this condition the 3BDAA model may provide a reasonable approximation of the full four-boson model for particular observables like the atom-trimer elastic scattering cross section and the tetramer position $(b_n - B_{n,0}^d)$, but not for reactions involving the dimer-dimer or lower atom-trimer channels. The intersection point estimations in Eqs. (3) and (4) refer to $|A_d|/a > 10^6$ and therefore should be reliable whereas the 3BDAA model fails for $a_{n,0}^t/a_n^d$ as can be seen in Fig. 2.

The tetramer lies very close to the atom-trimer threshold, even the largest deviation around $a_n^d/a = 0.8$ is only $(b_n - B_{n,0}^d)/b_n \approx 2.26 \times 10^{-4}$. For comparison, the difference between the atom-trimer and dimer-atom-atom thresholds at this point is $(b_n - b_d)/b_n \approx 8.86 \times 10^{-3}$. Note that in a narrow interval around $a = a_{n,0}^t$ the tetramer is slightly above the atom-trimer threshold, i.e., $B_{n,0}^d < b_n$. The width $\Gamma_{n,0}^d$ vanishes at $a = a_{n,0}^t$ while at $a > a_{n,0}^t$ the $(n,0)$ th tetramer becomes an inelastic virtual state (IVS) [13]. Negative width $\Gamma_{n,0}^d < 0$ in the IVS case implies the change of the energy sheet. The IVS corresponds to the pole of the transition operators $\mathcal{U}_{\beta\alpha}$ in the complex energy plane on one of the nonphysical sheets that is, unlike the one of UBS, more distant from the physical sheet [13]. The IVS has a visible impact on the physical collision observables only when it is located very near to the scattering threshold [13]; an example referring to the four-boson system can be found in Ref. [14]. In contrast, the UBS always leads to a resonant behavior. As example we show in Fig. 3 the S -wave phase shift δ_S and inelasticity parameter η_S for the dimer-dimer and atom-trimer scattering at the total four-boson energy $E \approx -B_{n,0}^d$ and $a_n^d/a = 0.8$. It is interesting to note that only the dimer-dimer phase shift increases by 180 deg while the inelasticity parameter exhibits a rapid variation also for the collisions of atoms and trimers in the $(n-1)$ th Efimov state. Thus, in these two cases the inelastic reactions are significantly enhanced by the tetramer UBS whereas a pronounced resonant peak in the elastic cross section is present in the dimer-dimer channel only. The $(n,0)$ th tetramer has very little impact for the collisions of atoms and trimers in the $(n-2)$ th (and lower) Efimov state.

The $(n,0)$ th tetramer intersection with the n th atom-trimer threshold manifests itself most prominently in the atom collisions with the n th trimer at vanishing relative kinetic energy. The corresponding atom-trimer scattering length A_n is shown in Fig. 4 as a function of the two-boson scattering length a . A_n exhibits a resonant behavior with $|\text{Im } A_n|$ having a peak at $a = a_{n,0}^t$. The

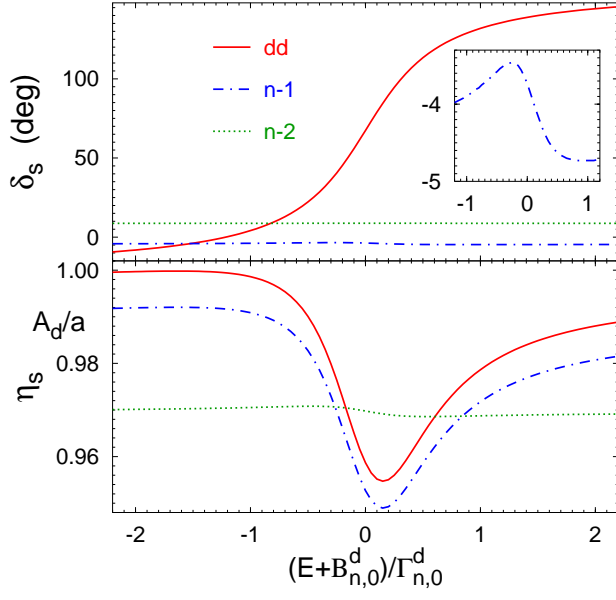


FIG. 3. (Color online) S -wave phase shift and inelasticity parameter for the dimer-dimer (solid curves) and atom-trimer scattering where the trimer is in the $(n-1)$ th (dashed-dotted curves) or in the $(n-2)$ th (dotted curves) Efimov state. The energy regime around the $(n,0)$ th tetramer state at $a_n^d/a = 0.8$ is shown.

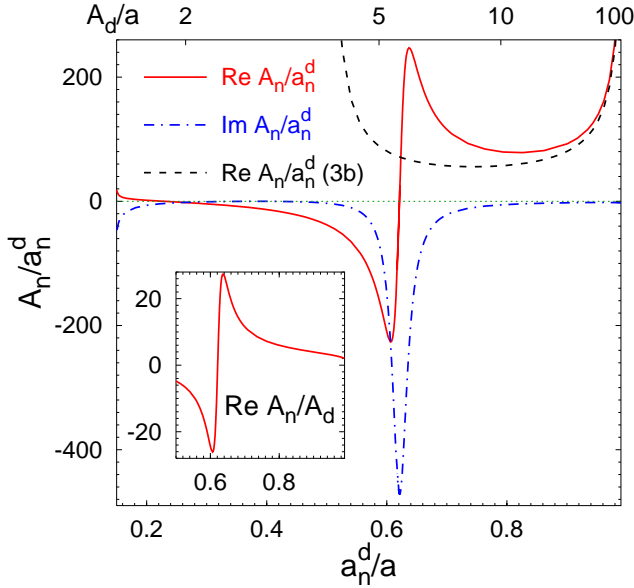


FIG. 4. (Color online) Real (solid curve) and imaginary (dashed-dotted curve) parts of the atom-trimer scattering length A_n as functions of the two-boson scattering length a and the atom-dimer scattering length A_d . Results for $\text{Re } A_n$ obtained using the 3BDAA model are shown as dashed curve. The thin dotted line represents the zero value.

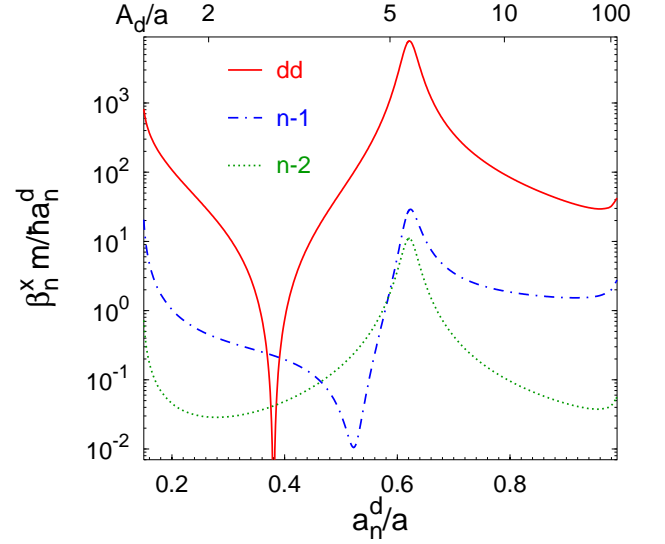


FIG. 5. (Color online) Inelastic reaction rates for vanishing relative energy atom scattering from the n th trimer as functions of the two-boson scattering length a or the atom-dimer scattering length A_d . Rates for the dimer production (solid curve) and the trimer relaxation to the $(n-1)$ th (dashed-dotted curve) and to the $(n-2)$ th (dotted curve) Efimov state are compared.

increase of $\text{Re } A_n$ shown in Fig. 4 near $a_n^d/a = 0.99$ is not related to the tetramers; it is due to the scaling of the elastic cross section with the spatial size of the trimer that grows with increasing A_d and decreasing $(b_n - b_d)$, i.e., $\text{Re } A_n \sim A_d \sim (b_n - b_d)^{-1/2}$. This is evident in the inset of Fig. 4 where the ratio $\text{Re } A_n/A_d$ exhibits no resonant behavior near $a_n^d/a = 0.99$. The inelastic reactions quantified by $\text{Im } A_n$ are not significantly enhanced by the increased size of the trimer. The failure of the 3BDAA model, especially for $\text{Im } A_n$ and the resonant peak position, can be expected based on Fig. 2 and its discussion. We show in Fig. 4 the 3BDAA prediction only for $\text{Re } A_n$ at larger A_d/a values. Only at $A_d/a > 50$, i.e., $a_n^d/a > 0.96$, it agrees with the four-boson result within 7% or better. In the same regime the 3BDAA model underpredicts $\text{Im } A_n$ almost by a factor of 40 as compared to the four-boson result. As estimated in Eq. (4) using the 3BDAA model, the A_n resonance due to the $(n,1)$ th tetramer is expected to take place much closer to $a = a_n^d$. Finally we note that rapid variations of A_n near $a_n^d/a = 0.15$ are caused by the proximity of the dimer-dimer threshold and the Efimov tetramer (of a different type) that intersect the n th atom-trimer threshold at $a_n^d/a = 0.14730(1)$ [16] and $a_n^d/a = 0.14706(1)$ [14], respectively. The A_n evolution at $a_n^d/a < 0.15$ is presented in Ref. [14].

The inelastic reaction rate for the atom scattering from the n th trimer in the ultracold limit is given [9] by $\beta_n = -(16\pi\hbar/3m)\text{Im } A_n$ where m is the boson mass. β_n has contributions corresponding to the dimer production β_n^{dd} and the trimer relaxation $\beta_n^{n'}$ to more deeply

bound states n' , i.e.,

$$\beta_n = \beta_n^{dd} + \sum_{n'=0}^{n-1} \beta_n^{n'}. \quad (5)$$

The respective dimensionless quantities $\beta_n^{dd}m/\hbar a_n^d$ and $\beta_n^{n'}m/\hbar a_n^d$ are compared in Fig. 5. Consistently with our previous findings for two-cluster collisions [9, 16] and four-atom recombination [17], in most of the considered regime the dominating inelastic reaction is the one leading to the most weakly bound final channel, i.e., the dimer-dimer channel in the present case. However, in a narrow interval around $a_n^d/a = 0.38$ an interesting and unusual situation takes place: the dimer production rate β_n^{dd} is strongly suppressed and the trimer relaxation process becomes the most important inelastic reaction. Another exceptional situation can be seen around $a_n^d/a = 0.52$ where β_n^{n-1} has a minimum such that $\beta_n^{n-1} < \beta_n^{n-2}$.

The considered regime is not yet explored experimentally. According to our predictions, the $(n,0)$ th tetramer most clearly could be seen as a dimer production rate peak in ultracold collisions of atoms and excited trimers in the n th state, since $a_{n,0}^t$ is quite well separated from other special values of a . Of course, in real experiments the resonance position may deviate from the universal value (2) due to finite-range effects; however, even without the dimer-trimer intersection, i.e., without the a_n^d point in Fig. 1, the tetramer may still exist as it happens in our model with $n = 1$. On the other hand, the observation of the resonant behavior in elastic or inelastic dimer-dimer collisions requires a very fine energy resolution since the tetramer lies very close to the atom-trimer threshold. The situation is even more complicated if deeply bound dimer states are present such that the Efimov trimers become UBS with finite width and lifetime. According to Ref. [3], the trimer width is of the order $\eta_* b_n$ with η_* being the atom-dimer inelasticity

parameter; for example, $\eta_* \approx 0.03$ in the experiment of Ref. [21] performed at $a > 0$ and $\eta_* \approx 0.1$ in the experiment of Ref. [19] performed at $a < 0$. Thus, the width of the trimer greatly exceeds the distance $(B_{n,0}^d - b_n)$ between the tetramer and the atom-trimer threshold, such that from the experimental point of view the n th trimer and the $(n,0)$ th tetramer are on top of each other. Furthermore, in the presence of deep dimers the atom-dimer scattering length A_d is complex with finite real and imaginary parts. For example, $|\text{Re } A_d/a| < 40$ at $\eta_* \approx 0.03$ [3]. This should be sufficient for the existence of the $(n,0)$ th tetramer at a slightly above a_n^d but excludes all the others $(n, m \geq 1)$. For larger η_* values even the $(n,0)$ th tetramer may be absent. Thus, the experimental observation of the considered tetramers would be extremely difficult.

IV. SUMMARY

We studied bosonic tetramers that have approximate dimer-atom-atom structure. They are unstable bound states in the continuum affecting the scattering processes in the four-boson system. Exact four-particle equations for the transition operators were solved in the momentum-space framework to describe the four-boson collisions. We accurately achieved the universal limit by considering reactions involving highly excited trimers but, for a given trimer, the results are restricted to the deepest tetramer only. We calculated the atom-trimer and dimer-dimer scattering observables to extract the tetramer position and width. In particular, we determined the tetramer intersection with the atom-trimer threshold and demonstrated that in ultracold atom-trimer collisions it leads to a resonant enhancement of elastic and inelastic reactions. We studied also the reliability of the three-body dimer-atom-atom model for the atom-trimer collisions: it may be reasonable for the elastic scattering near threshold and the real part of the tetramer energy at $|A_d| \gg a$ but fails for the inelastic reactions and the tetramer width.

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